

Pentaerythritol  
115-77-5 | DTXSID2026943

Model Performance

Model	Data
-------	------

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 8.70 L/kg

Global applicability domain: Inside

Local applicability domain index: 4.17e-01

Confidence level: 5.44e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Maleic hydrazide</div> <div>Measured: 2.82</div> <div>Predicted: 5.12</div>	<div>Image not found</div> <div>Diethanolamine</div> <div>Measured: 3.98</div> <div>Predicted: 4.00</div>	<div>Image not found</div> <div>6-Methyl-2-thiouracil</div> <div>Measured: 138</div> <div>Predicted: 99.5</div>
<div>Image not found</div> <div>Amitrole</div> <div>Measured: 17.8</div> <div>Predicted: 10.6</div>	<div>Image not found</div> <div>1-Methoxy-2-propyl acetate</div> <div>Measured: 2.29</div> <div>Predicted: 7.33</div>	